Irreversibility of infinite range spin glasses

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By employing the "slow-cooling" iterative solution of the mean field equations, we study the free energy surface of the isotropic, infinite range Ising and Heisenberg spin glasses with up to 800 spins. Ising model results for the field cooled and zero field cooled magnetizations as well as the magnetic hysteresis loops are similar to those found for the short ranged model. However, the results for the Heisenberg model depend strongly on the range of the interaction. The infinite range model shows macroscopic irreversiblity, in contrast to the short range isotropic Heisenberg case which has no irreversibility.

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The infinite range spin-glass model described by Sherrington and Kirkpatrick[1] (SK) provides a useful starting point for a theory of spin glasses. Despite considerable effort, little progress has been made in developing a satisfactory microscopic theory of spin glasses.[2] Much of our present understanding comes from numerical analysis of simplified models.[2] While some progress has recently been made in understanding the nonergodic[3–6] behavior of the infinite-range Ising spin glass, there has been little work on the irreversible and time dependent properties of this model. Theoretical studies[7,8] of the infinite range isotropic Heisenberg model using replica techniques find a spin glass phase at a well-defined transition temperature T_c. Below T_c, it has been shown that this replica symmetry is broken. Though the breaking of replica symmetry is often presumed to be related to irreversibility and the onset of history dependent effects, there is presently no proof that these phenomena are connected. In this paper, we explore the irreversible and metastable properties of both the Ising and Heisenberg infinite range spin glasses.

Recently, it was demonstrated[9–11] that the minima of the free energy surface as functions of temperature T and external field H could explain the nature of reversibility and irreversibility in *short-range* Ising and Heisenberg spin glasses. One very striking result[10] is that in an *isotropic* Heisenberg spin glass, there is no irreversibility. The field-cooled (FC) and zero-field-cooled (ZFC) states are the same and magnetic hysteresis is absent. These results at first sight seem to be in conflict with those of Refs. 7 and 8, if we make the (as yet unproved) connection between replica symmetry breaking and the onset of irreversibility. However, since the calculations of Refs. 7 and 8 are for an infinite-range model, it is important to study within the free energy formalism the reversibility or irreversibility of the long-range models.

In the present paper we report results for the FC and ZFC magnetizations and magnetic hysteresis for both the Ising and Heisenberg infinite range spin glasses. We employ the iterative mean field theory for our calculation which at $T = 0$ is equivalent to that used in Monte Carlo calculations for obtaining ground states. However, our iterative mean field approach is a factor of 10–100 times faster which enabled us to determine for the first time the ground state energy and the internal field distribution for the infinite range Heisenberg spin glass.[11]

The SK model generalized to vector spins is described by the Hamiltonian

$$\mathscr{H} = -\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{H}\cdot\mathbf{S}_i \tag{1}$$

for N classical spins S_i where H is the external magnetic field. The summation is over all pairs (i,j). The exchange interactions J_{ij} are given by a Gaussian distribution of mean $J_0/(N-1)$ and variance $J^2/(N-1)$. We take $J = 1$. The N dependence of the interactions ensures a correct thermodynamic limit. The spins are an m-component vector, except for $m = 1$ which is Ising-like.

In these calculations, we look at the simplest mean field model for the free energy functional $F[m_i]$, where m_i is the thermal average of the spin at the ith site. The corrections to mean field theory, deriving from the "reaction term" lead to unphysical results. Since, in the short-ranged models, the simple mean field theory has led to useful insights, we shall adopt that method here. It is important to note that the ground states ($T = 0$) derived in mean-field theory satisfy the condition for metastability used in Monte Carlo simulations.

For the vector spin glasses, we solve iteratively the self-consistent equations deriving from $dF/d\mathbf{m}_i = 0$,

$$\mathbf{m}_i = \mathbf{h}_i S B_S(|h_i|)/|h_i| , \tag{2a}$$

where $\mathbf{h}_i = \beta\mathbf{H} + \beta\Sigma_j J_{ij}\mathbf{m}_j$ and B_S is the Brillouin function for general spin S and $\beta = 1/kT$. We choose $S = 1$ for the Heisenberg model. To be consistent with previous calculations for the Ising model,[1,3] we consider $S = \pm 1$,

$$m_i = \tanh\beta\left(\sum_j J_{ij}m_j + H\right). \tag{2b}$$

Convergence is assumed when

$$\sum_i [(\mathbf{m}_i)_n - (\mathbf{m}_i)_{n-1}]^2 \Big/ \sum_i (\mathbf{m}_i)_n^2 \leqslant 10^{-8} , \tag{3}$$

where the subscript n denotes the nth iteraction. Our results are essentially unchanged if we choose a less stringent error criterion, say 10^{-6}. However, for any weaker convergence criterion, we observe significant differences in the final results for the energy, free energy, and magnetization. In most cases we begin our numerical calculations at $T > T_c$ where T_c is the mean field spin glass transition temperature and cool in zero or finite field. We put $\mathbf{m}_i$ in a randomly chosen direction at high T and decrease T in small steps, typically 0.1 or 0.2 J. At each T we can follow the solution with decreasing T without difficulty. At each subsequent T, the converged values of the previous temperature is used to start the next interaction. In this way it is assumed that the system "follows" a given minimum of the energy surface as it evolves with H and T. As in most numerical approaches, we take advantage of the fact that updating the $\mathbf{m}_i$ as we iterate leads to much more rapid convergence.

ISING MODEL RESULTS

The Edwards–Anderson order parameter $Q = \Sigma_i m_i^2 / N$ as a function of T for three different system sizes N is qualitatively similar to the short range results.[9,10] T_c is defined as the lowest T at which $Q = 0$, obtained by extrapolating to $N \to \infty$. From our numerical results we get $T_c \approx 2$ J, consistent with the exact result for the mean field equations, Eq. (2b). Note this value for T_c is twice the exact value for the infinite range Ising model. It is interesting to note that if we plot Q as a function of T/T_c where $T_c = 2$ J, the results agree well with the Q obtained from Monte Carlo studies.[1] 2J is also the value at which the ZFC magnetization $M^{\rm ZFC}$ has a maximum for small H. In Fig. 1 we plot the temperature dependence of $M^{\rm ZFC}$ and $M^{\rm FC}$ (corresponding to the lower and upper curves respectively, for each pair of curves). The values of the magnetic field (in units of J) are indicated. These results are an average over 50 bond configurations for $N = 200$ spins. An average of 100 configurations for 100 spins gives qualitatively the same result. From Fig. 1 it is evident that the results for FC and ZFC magnetization for the infinite range Ising spin glasses are similar with those of the Ising short range model.[9] The arrows in the bottom sets of curves of Fig. 1 indicate that the ZFC curve is obtained upon warming only. The FC curve, by contrast, is completely reversible with respect to temperature variations. As the field increases, the splitting of the FC and ZFC curves decrease. This is a direct reflection of the fact that the number of minima on the free-energy surface decreases as H increases. In Fig. 2 we plot for different H the temperature at which the $M^{\rm FC} = M^{\rm ZFC}$, i.e., the T below which irreversibility sets in.

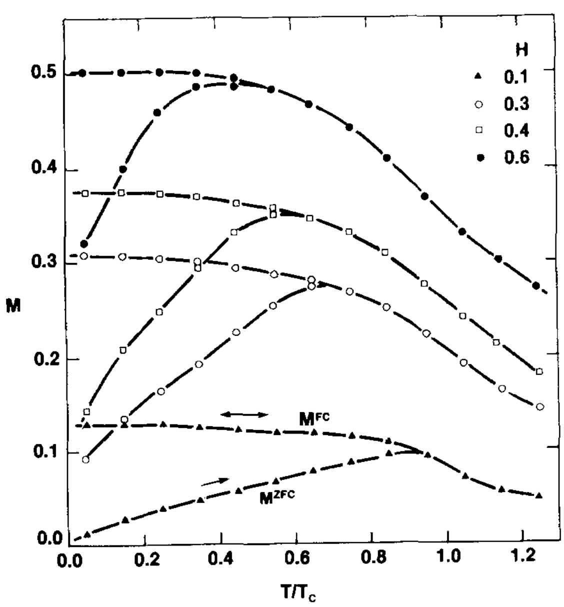

FIG. 1. Temperature dependence of field-cooled (FC) and zero-field-cooled (ZFC) magnetization for $N = 200$ averaged over 50 samples for various magnetic fields H (in units of J). $T_c = 2$ J.

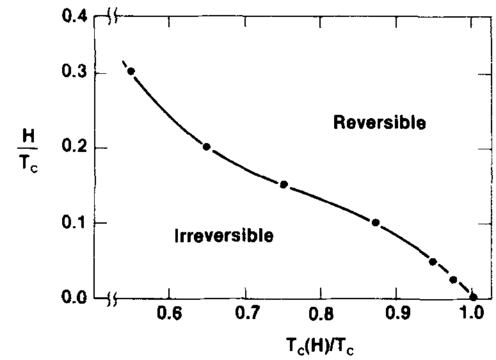

FIG. 2. Dependence of the reduced field H/T_C on the reduced temperature $T_c(H)/T_c$. $T_c(H)$ is the T at which $M^{\rm FC} = M^{\rm ZFC}$, and $T_c \equiv T_c(0)$.

We also studied the magnetic hysteresis for very low T, shown in Fig. 3 for $J_0 = 0.0$ and 0.50. The results are averaged over 50 configurations for $N = 200$. As expected as J_0 increases the magnetic hysteresis loops become sharper.

All of our results for the infinite range Ising model agree with our previous results for the short range model.[9] However, it is interesting that for the infinite range model, it is possible to construct a Hamiltonian[12] for which the mean field equations, Eq. (3), are exact. This new Hamiltonian can be solved exactly using replica techniques and the results compared with our numerical results. This should be an interesting test of the replica symmetry breaking methods. This work is in progress and will be reported separately.

HEISENBERG MODEL RESULTS

Our previous results for the infinite range Heisenberg spin glass indicated that unlike the short ranged models the

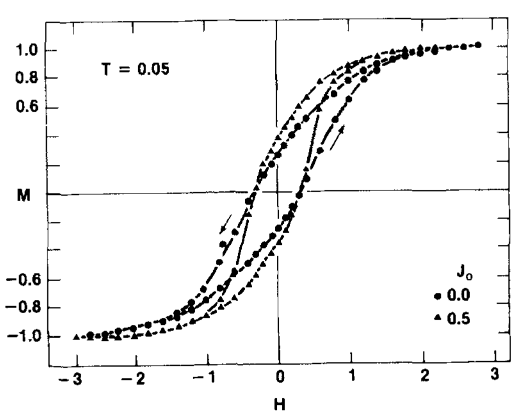

FIG. 3. Magnetic hysteresis curves M vs H, for symmetric field sweeps from high field for $N = 200$ averaged over 50 samples at $T = 0.05$ for two values of J_0. All energies are measured in units of J.

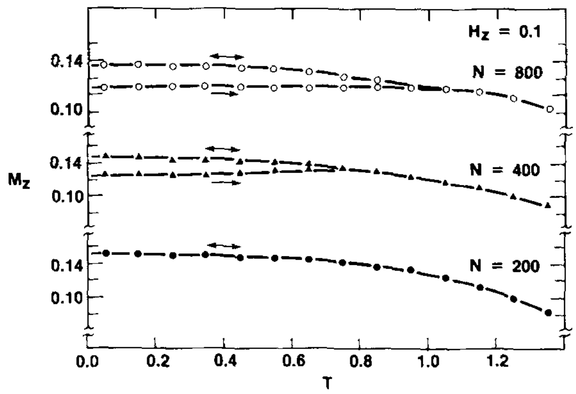

FIG. 4. Temperature dependence of field-cooled (FC) and zero-field-cooled (ZFC) magnetizations for the isotropic, Heisenberg infinite range spin glass system for different N and $H_z = 0.1$.

system showed signs of macroscopically irreversible for $N \gtrsim 400$ spins. We have systematically studied this irreversibility in the infinite range model. By cooling in the presence of a small magnetic field ($H = 0.1$), we can calculate $M^{\rm FC}$. However, by slowly cooling from high T to very low T in the presence of zero external field and then applying the field, we calculate $M^{\rm ZFC}$. For $N \leqslant 200$ spins there is no irreversibility ($M^{\rm FC} = M^{\rm ZFC}$) but for $N \gtrsim 400$, the system is irreversible ($M^{\rm FC} \neq M^{\rm ZFC}$). This is clearly shown in Fig. 4 where we plot the FC and ZFC magnetizations for $H = 0.1$ for three values of N. We averaged over 15, 7, and 4 configurations for $N = 200, 400$, and 800, respectively. Note that as N increases the splitting of the FC and ZFC curves increases. We also examine FC and ZFC magnetizations for 800 spins for different magnetic fields. For a small external magnetic field $M^{\rm ZFC}$ is qualitatively different than we found the Ising model. Here $M^{\rm ZFC}$ remains flat as a function of T, always smaller than $M^{\rm FC}$. Only at higher T does $M^{\rm ZFC}$ meet $M^{\rm FC}$. As H increases, the splitting decreases. At $H_z = 0.4$, $M^{\rm FC} = M^{\rm ZFC}$.

In conclusion, we note that the most important aspect of the present work is that irreversibility exists for the infinite range Heisenberg spin glass. We find that the range of interaction plays an important role in determining the irreversible behavior of the Heisenberg spin glasses. It seems that the barriers between minima become larger as the range of interaction increases and the lowest energy state is not as accessible as in the finite range case.

ACKNOWLEDGMENT

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[1]D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35**, 1792 (1975); Phys. Rev. B **17**, 4384 (1978).
[2]For a recent review see K. H. Fischer, Phys. Status. Solidi B **116**, 357 (1983).
[3]A. P. Young and S. Kirkpatrick, Phys. Rev. B **25**, 440 (1982); A. P. Young and S. Jain, J. Phys. A **16**, L199 (1983).
[4]H. Sompolinsky, Phys. Rev. Lett. **47**, 935 (1981).
[5]N. D. Mackenzie and A. P. Young, Phys. Rev. Lett. **49**, 301 (1982).
[6]F. T. Bantilan and R. G. Palmer, J. Phys. F **11**, 261 (1981).
[7]M. Gabay and G. Toulouse, Phys. Rev. Lett. **47**, 201 (1981).
[8]D. M. Cragg, D. Sherrington, and M. Gabay, Phys. Rev. Lett. **49**, 158 (1982).
[9]C. M. Soukoulis, K. Levin, and G. S. Grest, Phys. Rev. Lett. **48**, 1756 (1982); Phys. Rev. B **28**, 1495 (1983).
[10]C. M. Soukoulis, G. S. Grest, and K. Levin, Phys. Rev. Lett. **50**, 80 (1983); Phys. Rev. B **28**, 1510 (1983).
[11]G. S. Grest and C. M. Soukoulis, Phys. Rev. B **28**, 2886 (1983).
[12]A. J. Bray (private communication).